

Luttinger liquid phenomenology and angle resolved photoemission for single layer $\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ high-temperature superconductor

K. BYCZUK¹, C. JANOWITZ², R. MANZKE², J. SPAŁEK³, and W. WÓJCIK⁴

¹ *Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, 00-681 Warszawa, Poland*

² *Humboldt Universität, Institute für Physik, Newtonstr. 15, 12489 Berlin, Germany*

³ *Institute of Physics, Jagiellonian University, ul. Reymonta 4, 30-059 Kraków, Poland*

⁴ *Institute of Physics, Cracow University of Technology, ul. Podchorążych 1, 30-084 Kraków, Poland*

(received ???; accepted ???)

PACS. 74.72.-h – Cuprate superconductors.

PACS. 74.72.Hs – Bi-based cuprates.

PACS. 79.60.-i – Photoemission and photoelectron spectra.

PACS. 71.10.Hf – Non-Fermi-liquid ground states.

Abstract. – Recently observed splitting in angular resolved photoemission spectroscopy (ARPES) on $\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ high-temperature superconductor (Janowitz C. *et al.*, *Europhys. Lett.*, **60** (2002) 615) is interpreted within the phenomenological Luttinger-liquid framework, in which both the non-Fermi liquid scaling exponent of the spectral function and the spin-charge separation are introduced. The anomalous Green function with adjustable parameters fits very well to the Fermi edge and the low-energy part of ARPES along the $\Gamma - M$ line in the Brillouin zone. In contrast to one-dimensional models with Luttinger-liquid behavior we find that both the anomalous scaling α and the parameter δ describing the spin-charge separation are momentum dependent. The higher-energy part of the spectra is not accounted for by this simple Luttinger-liquid form of the Green function. In this energy regime additional scattering processes are plausible to produce the experimentally observed wide incoherent background, which diminishes as the inverse of the energy.

The understanding of physical properties of high-temperature superconductors and, in particular, of their normal phase properties, is a notoriously difficult problem for more than 15 years. The absence of the Fermi-liquid *quasiparticles* in the normal state at the optimal doping or in the underdoped regime, that was concluded on the basis of thermal, photoemission, or transport experiments [1], has given rise to the search for a *non-Fermi liquid theory* of high-temperature superconductors [2]. Despite of many microscopic and phenomenological approaches, the problem of finding the theory for high-temperature superconductors has not yet been resolved.

In a microscopic approach to many-body systems one investigates suitable correlation functions, usually within the renormalized perturbation scheme [3]. From these functions

physical properties of the system are determined and compared with experimental results. In a macroscopic (phenomenological) approach one starts with a certain expression for either the thermodynamic potential (e.g. from a Ginzburg-Landau functional [4]) or correlation function [5, 6], which have adjustable parameters that are fixed by fitting the results to experimental data. Only in a limited number of cases the macroscopic approaches are traced back to microscopic theories. Nevertheless, the power of the phenomenological approach lies in its ability to explain physical properties of real materials and, sometimes, allows one to guess some features of the albeit unknown microscopic approach.

In the macroscopic *Fermi liquid* theory the proper single-particle excitations are the *quasi-particles*, which remain in one-to-one correspondence with the states of noninteracting electrons and turn out to be the exact single-particle excitations near the Fermi surface at zero or low temperatures. In the microscopic theory these quasiparticles occur as single poles near the real axis on the complex energy plane in the retarded one-particle Green function $G(\mathbf{k}, \omega)$, where \mathbf{k} is a momentum and ω is an energy. These quasiparticles are seen as sharp peaks in the spectral function $A(\mathbf{k}, \omega) \equiv -(1/\pi)\text{Im}G(\mathbf{k}, \omega)$ appearing on the top of an incoherent background. The angular resolved photoemission spectroscopy (ARPES) data taken on one- and two-dimensional metallic systems can be interpreted as a direct probe of the spectral function $A(\mathbf{k}, \omega)$, multiplied by the Fermi-Dirac occupation function, and convoluted with the apparatus function. This experimental technique was used to show that TiTe_2 is a two-dimensional Fermi liquid [7].

The canonical example of the non-Fermi liquid theory is provided by the exactly solvable Tomonaga-Luttinger model of interacting electrons propagating in one spatial dimension. The one-particle Green function in that case does not have any poles representing the electron-like quasiparticles. Instead, it has *branch cuts* on the real energy axis and is characterized by a non-universal exponent α , which depends on the strength of the electron-electron interaction. Physically speaking, if a single electron is either injected into or emitted from this one-dimensional system, it gets fractionalized into the whole bunch of exact one-particle excitations of this system, the *holons* and the *spinons*, carrying respectively the charge and the spin. Such an electronic system is called the *Luttinger liquid*. The absence of quasiparticles in ARPES and the signatures of the spin-charge separation were reported in few experiments performed on effectively one-dimensional metallic compounds [8–10]. Recently, the spin-charge separation was suggested [11] in ARPES carried out on a two-dimensional high-temperature superconductor.

In the present Letter we investigate the ARPES data for $\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ high-temperature superconductor [11] within a *macroscopic* framework. Namely, we fit the proposed phenomenological the Luttinger-liquid Green function with few adjustable parameters to these data. We show that those data can be consistently interpreted within the Luttinger liquid approach, in which the spin-charge separation occurs. We find that the parameters appearing in the one-particle Green function are momentum dependent, which is in contrast to the one-dimensional Tomonaga-Luttinger model, where these parameters are universal. From this fitting procedure we determine the dispersion of the holons and the spinons. However, a high-energy-tail scaling as $1/\omega$ represents probably an incoherent background, which cannot be accounted for within our phenomenological scheme.

The one-particle Green function for a Luttinger-liquid state in higher space dimensions may be proposed in the following general form

$$G(\mathbf{k}, \omega) = g \frac{\omega_c^{\mu+\nu-1} e^{i\phi}}{(\omega - \epsilon_{\mathbf{k}}^c)^\mu (\omega - \epsilon_{\mathbf{k}}^s)^\nu}, \quad (1)$$

where $\epsilon_{\mathbf{k}}^c$ ($\epsilon_{\mathbf{k}}^s$) is the momentum (\mathbf{k}) dependent charge (spin) one-particle excitation dispersion

relation, μ and ν are \mathbf{k} -dependent anomalous scaling exponents in the Luttinger liquid theory, ω_c is the energy cutoff, ϕ is a phase to be fixed, and g is a normalization coefficient [12]. When $\epsilon_{\mathbf{k}}^c = \epsilon_{\mathbf{k}}^s$ the Luttinger–liquid Green function with only anomalous scaling is recovered [13]. If $\mu = \nu = 1/2$ the Luttinger–liquid Green function with only spin–charge separation is obtained. In the limit when both $\epsilon_{\mathbf{k}}^c = \epsilon_{\mathbf{k}}^s$ and $\mu = \nu = 1/2$, the expression (1) represents the Fermi liquid with no damping of the quasiparticle states. In general case, the exponents μ and ν and the phase ϕ are to be constrained by other fundamental assumptions.

As in the low–energy Fermi liquid theory with linearized dispersion relation, we assume that the spectral function obtained from (1) is particle–hole symmetric, i.e. $A(\mathbf{k}, \omega) = A(-\mathbf{k}, -\omega)$ [13]. Then, the following physically distinct cases should be considered: (i) $\mu = \nu = 1/2 - \alpha$ and (ii) $\nu = 1/2$ and $\mu = 1/2 - \alpha$, where $0 \leq \alpha \leq 1/2$ in both cases. In the case (i) both the holon and the spinon singularities on the complex energy plane diverge with the same exponent, which in turn leads to the same height of the two peaks appearing in the spectral function. The normal– and the superconducting–state properties of the Luttinger liquid corresponding to the case (i) were investigated in Ref. [12]. However, the recent ARPES experiment [11] has shown that the heights of the holon and the spinon peaks are significantly different, that is consistent with the case (ii), also studied in Ref. [14]. Guided by these experimental results, we choose the Luttinger–liquid Green function corresponding to the case (ii). In addition to the particle–hole symmetry, we postulate the absence of relevant and marginal interactions in the spin sector on the microscopic level. In result, the spinon dispersion relation is not renormalized, i.e. $\epsilon_{\mathbf{k}}^s = \epsilon_{\mathbf{k}}$, where $\epsilon_{\mathbf{k}}$ is the bare–band dispersion relation. The holon dispersion relation is renormalized by the interactions and we assume that $\epsilon_{\mathbf{k}}^c \equiv \delta(\mathbf{k})\epsilon_{\mathbf{k}}$, where $\delta(\mathbf{k}) \geq 1$ is a \mathbf{k} -dependent parameter measuring the magnitude of the spin–charge separation. Note that in the exact one–dimensional theory the parameters α and δ would not be momentum dependent.

Our phenomenological one-particle Green function can be rewritten in the form

$$G(\epsilon_{\mathbf{k}}, \omega) = \frac{\omega_c^{-\alpha} e^{i\phi}}{\sqrt{(\omega - \epsilon_{\mathbf{k}}^c)(\omega - \epsilon_{\mathbf{k}}^s)}} \frac{g(\alpha, \delta)}{(\omega - \epsilon_{\mathbf{k}}^c)^{-\alpha}}, \quad (2)$$

where now $\alpha = \alpha(\mathbf{k})$ is the anomalous \mathbf{k} -dependent *scaling exponent* in the Luttinger liquid theory. The particle–hole symmetry fixes the unknown phase factor at the value $\phi = -\alpha\pi/2$. The spectral function has then the form:

$$A(\epsilon, \omega) = \frac{g(\alpha, \delta)\omega_c^{-\alpha}}{\pi} \left\{ \sin\left(\frac{\pi\alpha}{2}\right) \left[\frac{\Theta(\omega - \epsilon_s)\Theta(\omega - \epsilon_c)}{(\omega - \epsilon_s)^{1/2}(\omega - \epsilon_c)^{1/2-\alpha}} + \frac{\Theta(\epsilon_s - \omega)\Theta(\epsilon_c - \omega)}{(\epsilon_s - \omega)^{1/2}(\epsilon_c - \omega)^{1/2-\alpha}} \right] + \right. \\ \left. \cos\left(\frac{\pi\alpha}{2}\right) \left[\frac{\Theta(\omega - \epsilon_s)\Theta(\epsilon_c - \omega)}{(\omega - \epsilon_s)^{1/2}(\epsilon_c - \omega)^{1/2-\alpha}} + \frac{\Theta(\epsilon_s - \omega)\Theta(\omega - \epsilon_c)}{(\epsilon_s - \omega)^{1/2}(\omega - \epsilon_c)^{1/2-\alpha}} \right] \right\}, \quad (3)$$

where $\epsilon_s = \epsilon \equiv \epsilon_{\mathbf{k}}$, $\epsilon_c \equiv \delta(\mathbf{k})\epsilon$, and $\Theta(x)$ is the Heaviside step function. We fix the cutoff at $\omega_c = 1$ eV to set the energy scale. Obviously, the results for $A(\epsilon, \omega)$ should not be dependent on the value of ω_c .

The ARPES intensity, within a constant transfer matrix–approximation, is given by the convolution

$$I(\omega) = I_0 \int d\omega' A(\epsilon, \omega') f(\omega'/kT) R(\omega' - \omega), \quad (4)$$

where T is the temperature, $f(x)$ is the Fermi function, and $R(\omega)$ is an apparatus resolution function assumed in the Gaussian form $R(\omega) = \exp(-\omega^2/2\sigma^2)/\sqrt{2\pi\sigma^2}$. The phenomenological parameters $\alpha(\mathbf{k})$ and $\delta(\mathbf{k})$ are determined by fitting $I(\omega)$ to the ARPES data for

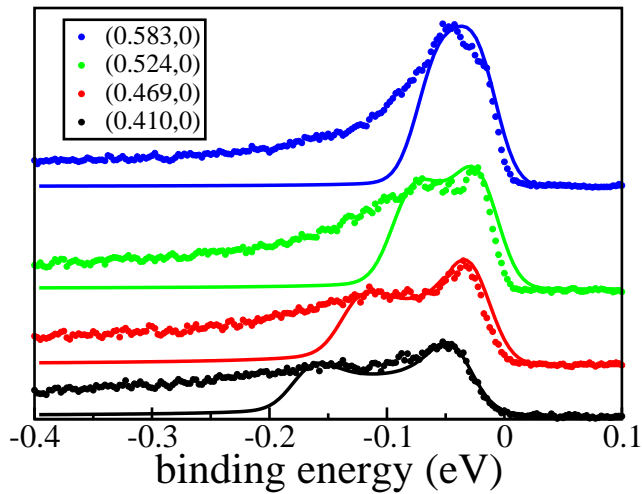


Fig. 1 – Selected ARPES data (dots) from Ref. [11] and the fitted spectral intensities (solid lines) within the Luttinger liquid phenomenology for different $|\mathbf{k}|$ vectors along $\Gamma - M$ direction of the Brillouin zone. The $|\mathbf{k}|$ vector values are in \AA^{-1} units.

$\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ compound with $x = 0.4$ for different values of the ARPES angle ϑ corresponding to different \mathbf{k} [11]. Also, the value of $\epsilon = \epsilon_{\mathbf{k}}$ for given \mathbf{k} is kept as a fitting parameter and thereby exempting us from additional assumptions on the hopping integral amplitudes within a tight-binding model of the electronic structure. We take $T = 35\text{ K}$ and $\sigma = 0.016\text{ eV}$ [11].

The $\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ high-temperature superconductor ($T_c = 29\text{ K}$ at the optimal doping $x = 0.4$) is a prototype of a system with a single CuO_2 layer. The large separation of the CuO_2 layers makes the system essentially two-dimensional in the normal state; no bilayer splitting of the band is expected. The occurrence of the two-peak structure in ARPES along the $\Gamma - M$ direction in the Brillouin zone [11] is interpreted as the Luttinger-liquid behavior in this system, as discussed below. The splitting cannot be attributed to the 1×4.8 superstructure of the CuO_2 planes, as the split bands obtained in this manner cannot be fitted to the experiment.

Selected ARPES data along $\Gamma - M$ $[(0,0) - (\pi,0)]$ direction in the Brillouin zone [11] and the fitted to them the intensity function $I(\omega)$, are shown in Fig. 1. As one can see, the Fermi edge region and the two-peak structure are very well reproduced by the spectral function form (3). The higher energy tails are not accounted for by our low-energy Luttinger-liquid Green function [15]. In Fig. 2 we provide the $|\mathbf{k}|$ dependence of the phenomenological parameters α and δ . The anomalous scaling exponent α is seen to decrease as one probes the system for higher \mathbf{k} values along the $(0,0) - (\pi,0)$ direction. The spin-charge separation parameter δ turns out to be non-monotonic function of \mathbf{k} having a maximum around the middle point of the $\Gamma - M$ line.

In Fig. 3 we plot the determined from the fitting dispersion relations $\epsilon_{\mathbf{k}}^c$ for holons and $\epsilon_{\mathbf{k}}^s$ for spinons along $\Gamma - M$ direction. Because of the interaction-induced renormalization, the holon excitations disperse more strongly than the spinons. These two *Luttinger-bands* are qualitatively similar to those obtained in [11], where they were represented by two separate Lorentzian spectral functions. A very small difference is found near the $(\pi,0)$ point, where

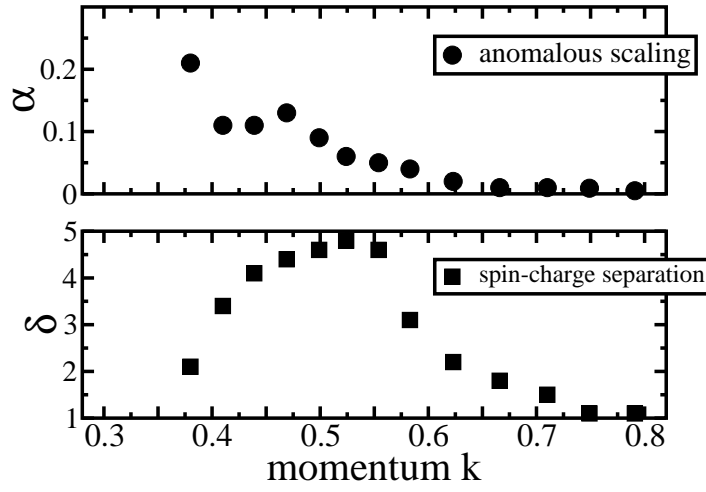


Fig. 2 – Anomalous scaling exponent $\alpha(\mathbf{k})$ (upper panel) and spin-charge separation parameter $\delta(\mathbf{k})$ (lower panel) as a function of momentum $|\mathbf{k}|$ (in \AA^{-1}) along the $\Gamma - M$ direction.

$\epsilon_k^c \approx \epsilon_k^s$ in our case. This difference might be caused only by a numerical uncertainty of the two procedures.

The presented comparison between the theory and the experiment allows us to conclude that the ARPES data on $\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ compound are consistent with the Luttinger liquid approach, in which *both the spin-charge separation δ and the anomalous scaling α are present at the same time*. This macroscopic investigation might also cast some light onto a possible microscopic theory of high-temperature superconductors. Namely, in the

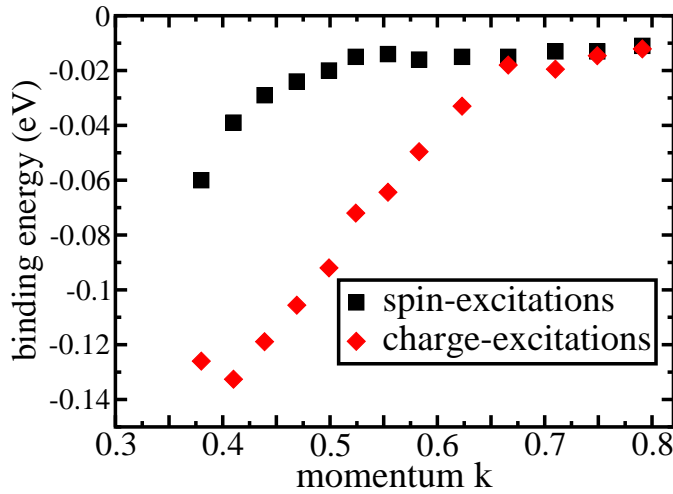


Fig. 3 – Dispersion relations for spinon (squares) and holon (diamonds) excitations along the $\Gamma - M$ direction.

one-dimensional systems of electrons interacting with short-range (screened) interaction, the Luttinger-liquid parameters α and δ were momentum independent. Here we find a significant momentum dependence of these parameters, that might suggest that the two-dimensional theory of the correlated liquid would be more complex. This conjecture is also supported by the absence of the spin-charge splitting in the ARPES data along $\Gamma - Y$ direction in the same compound [11]. In brief, one can say that the parameterization of the Green function – in terms of *branching cuts* (here) and in terms of *poles* (as in the Fermi liquid theory [16]) – represent two *complementary* ways of viewing this two-dimensional system: the former represents the extrapolation of the concept of quantum liquid from one dimension, whereas the latter utilizes the extrapolation of the concept of the Fermi liquid from three dimensions. It is tempting to say that this two-sided possibility of viewing the electronic states in CuO_2 planes means that the *lower critical dimensionality* for these system is $d_c = 2$.

Finally, we note that the phenomenological Green function (1) seems to describe only the low-energy part of the experimental spectra. The higher-energy spectral tails give almost one-half of the total spectral weight, as might be inferred from the fits in Fig. 1. Moreover, we note that this higher energy tails diminish as $A(\epsilon, \omega) \sim 1/\omega$, which is slower than the expected asymptotic decay of the one-particle spectral function for interacting fermions. We do not believe that the $1/\omega$ dependence represents the asymptotic high-energy tail when $\omega \rightarrow \pm\infty$ [3]. This is because the tail extends from $\omega \simeq 0.25 \text{ eV}$, i.e. from the energy range, where the intrinsic many-body dynamics is still very important. It is plausible that other scattering mechanisms, not present in the strictly one-dimensional theory, are responsible for this slow decay of holons, as well as for the broadening at higher energies. This observation cannot be quantified further within our phenomenological approach. Nonetheless, it might be used as an additional constraint in searching for the theory of high-temperature superconductivity.

In conclusion, we have presented the first quantitative analysis of photoemission spectra for the cuprates in terms of the Green function with branching cuts. The detailed analysis of the ARPES data for $\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ compound showed that they can be parameterized by a two-dimensional Luttinger liquid approach. This approach has still to be modified with respect to its one-dimensional correspondent to account for the high-energy part of the spectra. Also, the macroscopic parameters should be momentum dependent and additional scattering channels for the charge excitations should be added to the present approach.

* * *

Financial support of KB through the KBN Grant No. 2P03B 082 24 and of JS and WW through the KBN Grant No. 2P03B 050 23 is gratefully acknowledged. JS would like to thank the Foundation for Science (FNP) for a senior fellowship for the years 2003-6.

REFERENCES

- [1] For recent review see e.g. OTT H.R., in *The Physics of Superconductors*, edited by BENNEMANN K. H. and KETTERSON J. B., Vol. I (Springer, Berlin) 2003, p. 385ff.
- [2] ANDERSON P. W., in *Frontiers and Borderlines in Many-Body Physics, Proceedings of International School of Physics Varenna* (North Holland, Amsterdam) 1987; *The Theory of Superconductivity in the High- T_c Cuprates* (Princeton University Press, Princeton) 1997.
- [3] MAHAN G., *Many-Body Physics* (Plenum Press, New York) 1990.
- [4] See e.g. BLATTER G. and GESHKENBEIN V. B., Ref. [1], p.725ff.
- [5] INOUE I. H., HASE I., AIURA Y., FUJIMORI A., HARUYAMA Y., MARUYAMA T., and NISHIHARA Y., *Phys. Rev. Lett.*, **74** (1995) 2539.

- [6] BYCZUK K., BULLA R., CLAESSEN R., and VOLLHARDT D., *Int. J. Mod. Phys. B*, **16** (2002) 3759.
- [7] CLAESSEN R., ANDERSON R. O., ALLEN J. W., OLSON C. G., JANOWITZ C., ELLIS W. P., HARM S., KALNING M., MANZKE R., and SKIBOWSKI M., *Phys. Rev. Lett.*, **69** (1992) 808.
- [8] DENLINGER J. D., GWEON G. -H., ALLEN J. W., OLSON C. G., MARCUS J., SCHLENKER C., and HSU L. -S., *Phys. Rev. Lett.*, **82** (1999) 2540; *J. Phys. Chem. Solids*, **56** (1995) 1849; *Solid State Commun.*, **123** (2002) 469.
- [9] CLAESSEN R., SING M., SCHWINGENSCHLÖGL U., BLAHA P., DRESSEL M., and JACOBSEN C.S., *Phys. Rev. Lett.*, **88** (2002) 096402.
- [10] KIM C., MATSUURA A. Y., SHEN Z. -X., MOTOYAMA N., EISAKI H., UCHIDA S., TOHYAMA T., and MAEKAWA S., *Phys. Rev. Lett.*, **77** (1996) 4054.
- [11] JANOWITZ C., MÜLLER R., DUDY L., KRAPF A., MANZKE R., AST C. R., and HÖCHST H., *Europhys. Lett.*, **60** (2002) 615.
- [12] BYCZUK K., SPAŁEK J., and WÓJCIK W., *Acta Phys. Polonica B*, **29** (1998) 3871.
- [13] YIN L. and CHAKRAVARTY S., *Int. J. Mod. Phys. B*, **10** (1996) 805.
- [14] J. J. RODRIGUEZ-NUNEZ, I. TIFREA, and S. G. MAGALHAES, *Phys. Rev B*, **62** (2000) 4026; RODRIGUEZ-NUNEZ J.J., BUDAGODSKY J.A., and TIFREA M.I., *Acta Phys. Polonica*, **34** (2002) 383.
- [15] Thus the spectral intensity was fitted only to a part of the experimental spectra to describe properly the low-energy features. In effect, higher energy tail was simply excluded in the fitting procedure.
- [16] VARMA C. M., LITTLEWOOD P.B., SCHMITT-RINK S., ABRAHAMS E., and RUCKENSTEIN A.E., *Phys. Rev. Lett.*, **63** (1989) 1996.